PROJECT NUMBER: 0008
PROJECT TITLE: Computer Applications Division
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I. NEUROCOMPUTING

A. **Objective:** Develop programming techniques for use of the HNC ANZA Plus Neurocomputer and Multilayer Backpropagation Neurosoftware. Investigate potential applications of neurocomputing to R&D problems, and apply where appropriate.

B. **Results:** A new backpropagation neural network was developed for predicting liking scores from analytical data for menthol cigarettes. This network was trained on a training set of 1473 examples from both 85 mm and 100 mm smoking panels. The network incorporates 13 input variables - tar/puff, nicotine/puff, tipping, circumference, menthol/puff, and length for both the test cigarette and the smoker's preferred brand of choice, plus an additional variable for the type of 7-point liking scale. The standard error of the estimate is 0.43 on a 7-point liking scale. Based on predictions against a set of separate test data, the standard error of prediction is 0.49 on a 7-point liking scale.

The general purpose software tool, MBPN Tool, was significantly enhanced to improve the convergence of backpropagation learning. Principal enhancements include: (1) acceleration of learning rates on flat error surfaces, (2) adaptation of momentum terms for more stable and responsive learning, (3) reordering of examples between learning cycles to help avoid local minima, and (4) easier specification of training and testing data sets. These improvements should result in significantly faster convergence and fewer problems with local minima.

C. **Plans:** Using the new MBPN Tool, develop a new backpropagation network for predicting liking scores from analytical data for menthol cigarettes. Use this new network to perform sensitivity analyses to determine the effects of tar, nicotine/puff, menthol/puff, tipping, circumference, and length on liking.

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II. CIGARETTE INFORMATION EXPERT

A. **Objective:** Develop expert system for statistical analysis and interpretation of domestic cigarette information.

B. **Results:** The Cigarette Information Expert was prepared for delivery using the Nexpert Object Runtime Software.

C. **Plans:** Complete delivery of the Cigarette Information Expert. The software will reside and execute on a Sun Server, and will be accessed by personnel in CTSD through VT220 terminals.

III. EXPERT SYSTEMS DEVELOPMENT

A. **Objective:** Develop an Expert System for Cigarette Design.

B. **Results:** We have begun work on the third phase of our Cigarette Design Expert System (CigDES). The primary objective during this phase is to implement a knowledge-based ("heuristic") goal-directed reasoning capability. This new feature will provide a mechanism for resolving the "combinatorial explosion" problems characteristic of the "exhaustive" goal-directed reasoning process already implemented. The main component of the knowledge-based feature is a heuristic function which draws upon qualitative knowledge of cigarette performance to determine what design changes are most likely to lead to a cigarette prototype whose performance satisfies a set of user-defined goals. An initial algorithm for this heuristic function has been designed.

C. **Plans:** We will initially implement a heuristic function which selects cigarette design changes based only on causal relationships between design parameters and cigarette performance. We will then evaluate the heuristic goal-directed reasoning component of CigDES and, if its performance is not satisfactory, we will expand the qualitative model to provide more types of knowledge to the heuristic function.

IV GAS PHASE FIVE-PORT SMOKERS

A. **Objective:** Develop a new data acquisition system (DAS) for the five-port smokers in the CTSD) gas phase laboratory.

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B. **Results:** The Laser Precision Analytical FTIR instrument developed by Kent Koller has been moved to the CTSD Gas Phase Laboratory. Supplementary software for data computations and reporting for the CO, NO, Acetaldehydes, and HCN analyses has been completed and tested . The software for coordinating the operation of the Gas Phase five-port smoker in conjunction with the Laser Precision Analytical data acquisition and processing software is also completed and tested.

The software required to acquire and process Technicon Autoanalyzer Aldehyde and HCN data is being modified to improve the peak detection algorithm for Autoanalyzer data.

C. **Plans:** Software will be completed to support CO, NO, aldehyde, and HCN analyses by the autoanalyzer and FTIR technology.

D. **References:** CAD Project Request #3979

V HP GC CHEMSTATION UPGRADE FOR CTSD

A. **Objective:** Add software and hardware to the HP GC Chemstation to support bar code readers, setup for batchwise processing, post-run reporting and transfer of results to the CTSD LIMS database.

B. **Results:** Programming is complete. The software has been installed on the HP GC Chemstation and is undergoing evaluation.

C. **Plans:** Close out the project. Migrate the programs to other HP GC Chemstations as required.

D. **References:** CAD Project Request #4229

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